Plasma Opacities And High Precision Atomic Physics

LANL – EOS/Opacity V & V Workshop

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- Maximiliano Montenegro
- Brian Larkins
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- Werner Eissner – (Stuttgart)

Outline: Validity and Verification of EOS/Opacities

- "Academic" Perspective:
  → Accuracy AND Completeness
- Astrophysical opacities (OP and OPAL)
  → Current Problems: Radiative Accelerations
  New Solar abundances
- High Precision Atomic Physics
  → Theory and Experiment
- Monochromatic X-ray opacities
- Nanoscience and Nanotechnology
  → Biomedicine and Materials Research
- Plasma Fusion: ICF and Magnetic

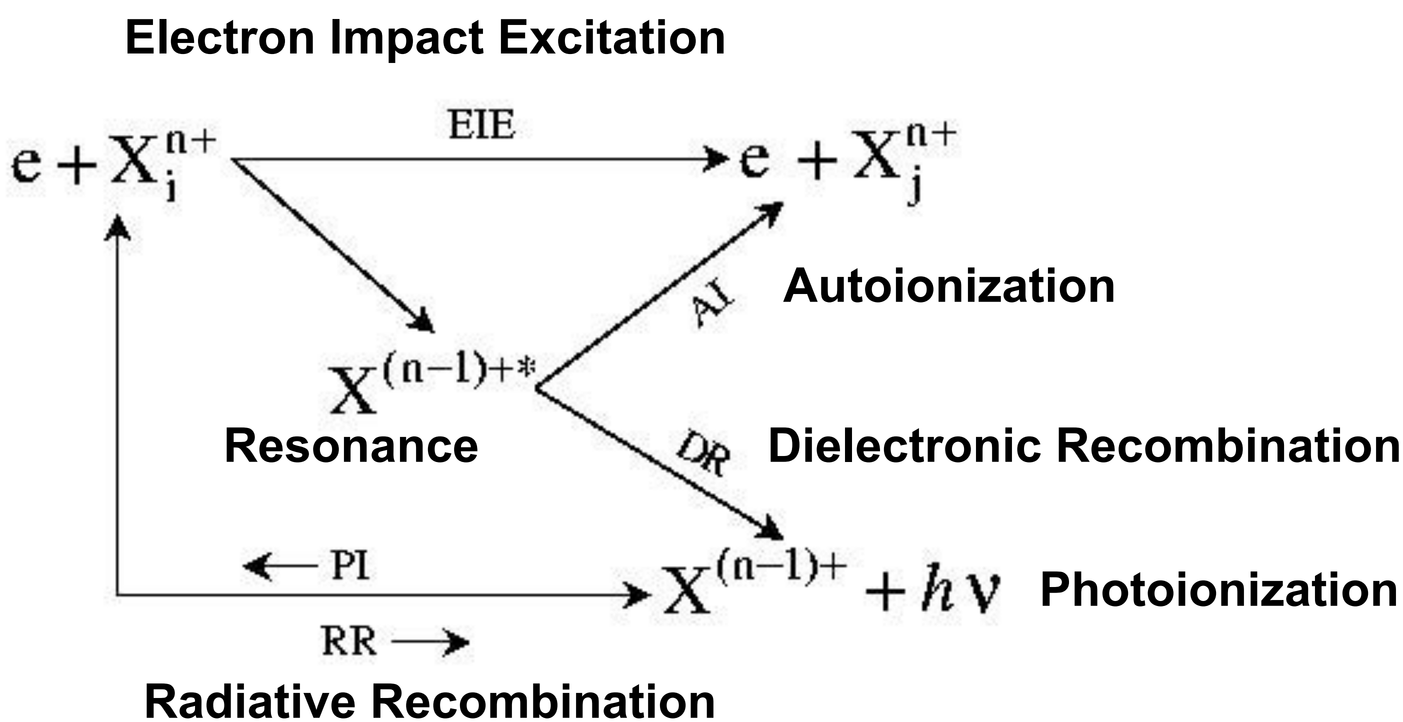
V &V – Academic Issues: Are we there yet?

- State-of-the-art atomic theory
- Continuous code development
- Study individual atomic processes in detail and compare with latest experiments (radiative transitions, photoionization, recombination, electron impact excitation)
- Large-scale calculations for laboratory and astrophysical opacities and spectral models

  → **The Opacity Project**

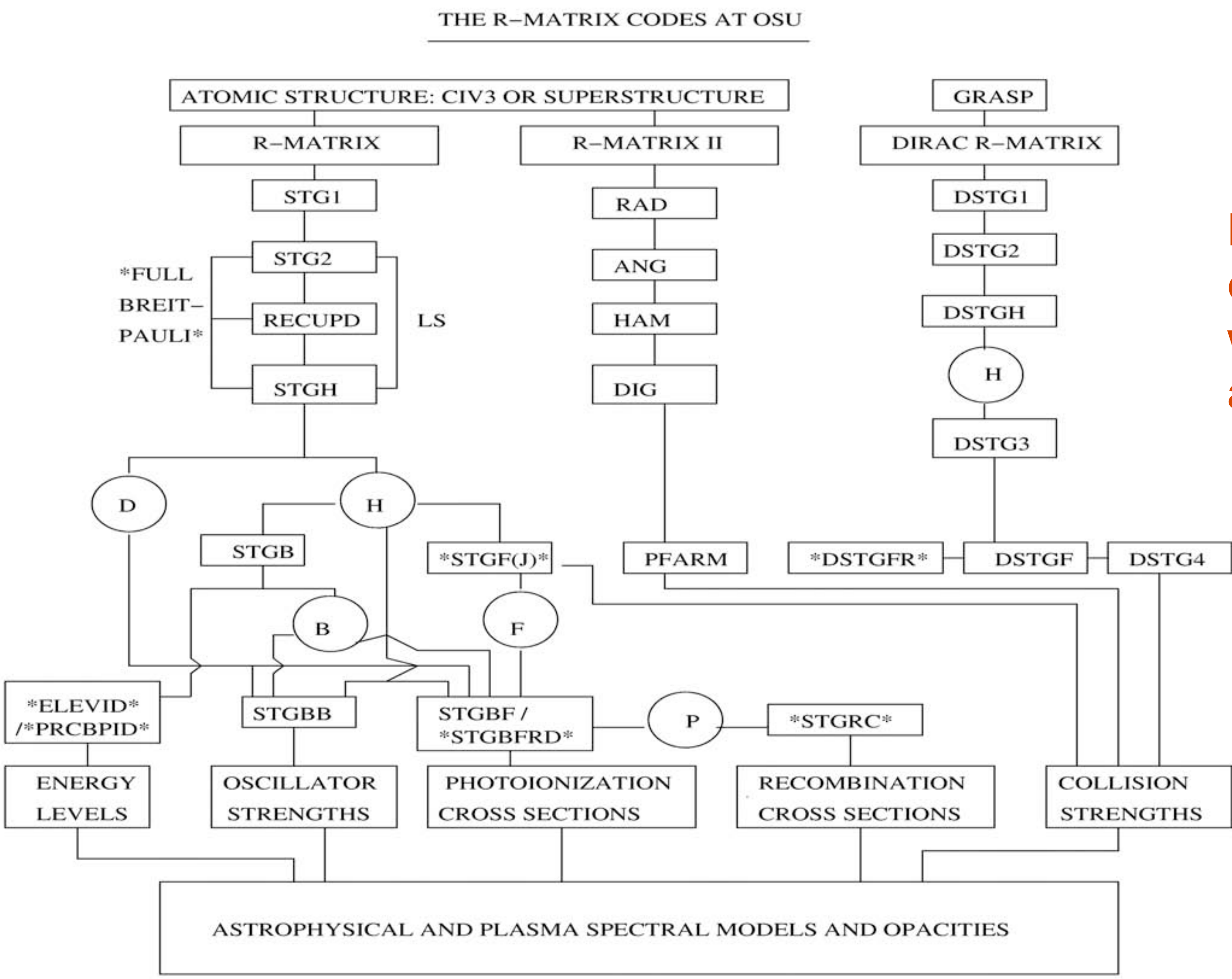
  → **The Iron Project (Fe-peak elements)**

Primary Atomic Processes in Plasmas



The Coupled-Channel R-matrix method provides a self-consistent and unified treatment of all processes with one single wavefunction expansion

Relativistic and Non-Relativistic R-matrix Codes For Atomic Processes (Ohio Supercomputer Center)



Large-scale calculations with high precision and self-consistency

The Opacity Project: Two independent sets of opacity codes for V&V

(i) M.J. Seaton, & Co., (ii) Yu, Mihalas, & Pradhan

Only (i) employed for final OP tabulations

The Opacity Project: 1983-2005

- Inception: 1983 → Group of > 30 researchers, 5 countries
  UK, US, France, Germany, Venezuela
- Cr, Mn, Ni – Extrapolation + Kurucz
- First complete results 1994 → OP1
  (Seaton, Yu, Mihalas, Pradhan, MNRAS, 266, 805, 1994)
- OP1 results for stellar **envelope** opacities;
  did **not** include
  → inner-shell processes
  → stellar interior EOS for $\rho > 0.01$ g/cc
- New OP work includes both
- On-line calculations for arbitrary composition
  → http://www.osc.edu/hpc/opacities
- CD-ROM from Anil Pradhan or Claude Zeippen

Astrophysical Opacities: The Opacity Project (OP) and LLNL (OPAL)

- The OP work used a combination of R-matrix and atomic structure calculations for bound-bound and bound-free
- Mihalas-Hummer-Dappen (MHD) EOS
- New OP work uses “extended” MHD-EOS
  - → High-density uncertainties
  - → Perturbed atom approximation
- Atomic data for inner-shell processes
  - → K-, L-, shell opacity

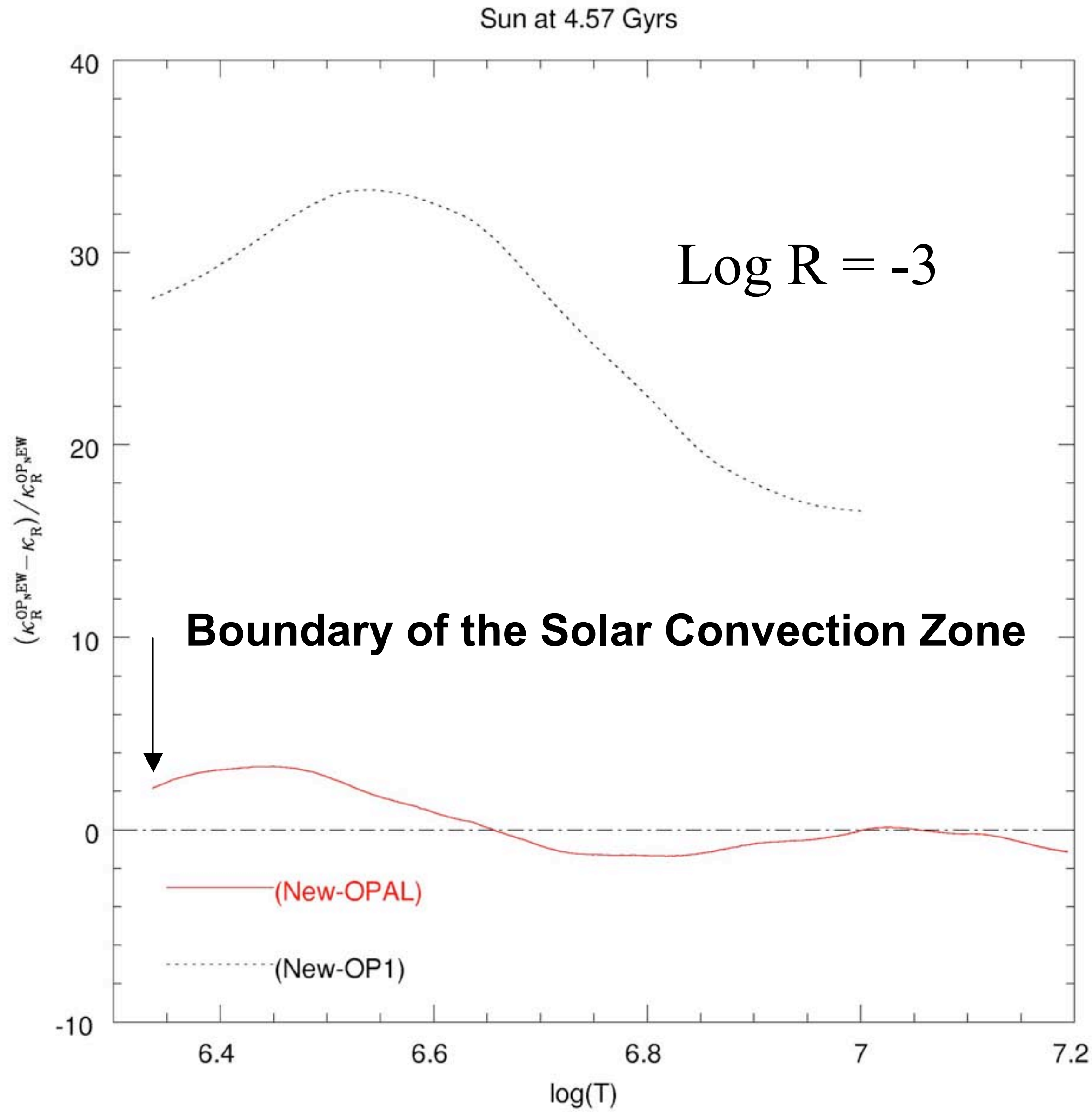
Astrophysical Opacities – Validation and Verification

- New OP and OPAL agree in the MEAN opacities at the 5-10% level
- But radiative accelerations disagree by factors of 2-5 !!

  → Monochromatic opacity resolution

  → Atomic physics accuracy
- V&V using Solar models similar in EOS, composition, central temperature, density, base of convection zone → very small differences

OP vs. OPAL → % Differences in Rosseland Mean Opacities



Delahaye & Pinsonneault (2005, ApJ in press)

OP1
Envelope EOS only, and Without Inner-shell Processes

New
Extended EOS, and including Inner-shell Processes
(Badnell et.al. 2005)

The Opacity Project (OP) and the OPAL Rosseland Mean Opacities

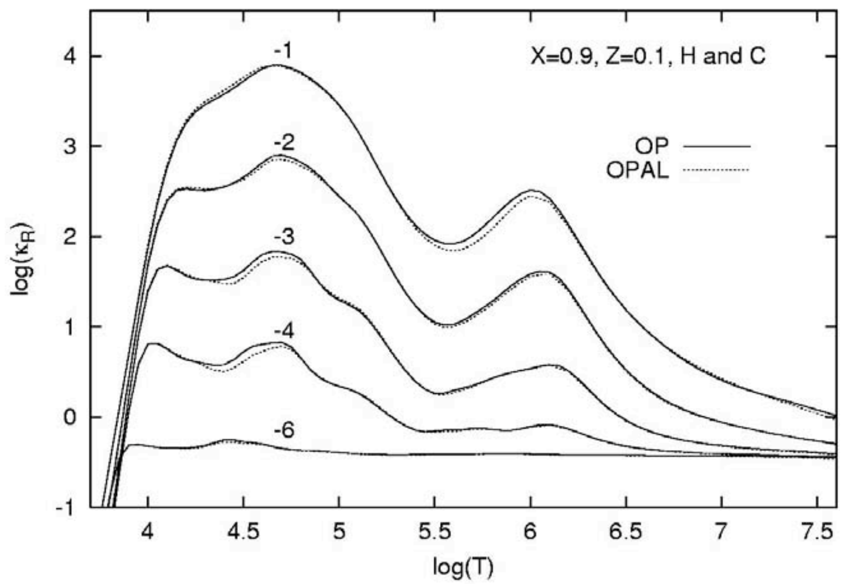


Figure 5. Comparisons of $\log(\kappa_R)$ from OP and OPAL for a H/C mixture with mass fractions $X = 0.9$ for H and $Z = 0.1$ for C. Curves are labelled by values of $\log(R)$.

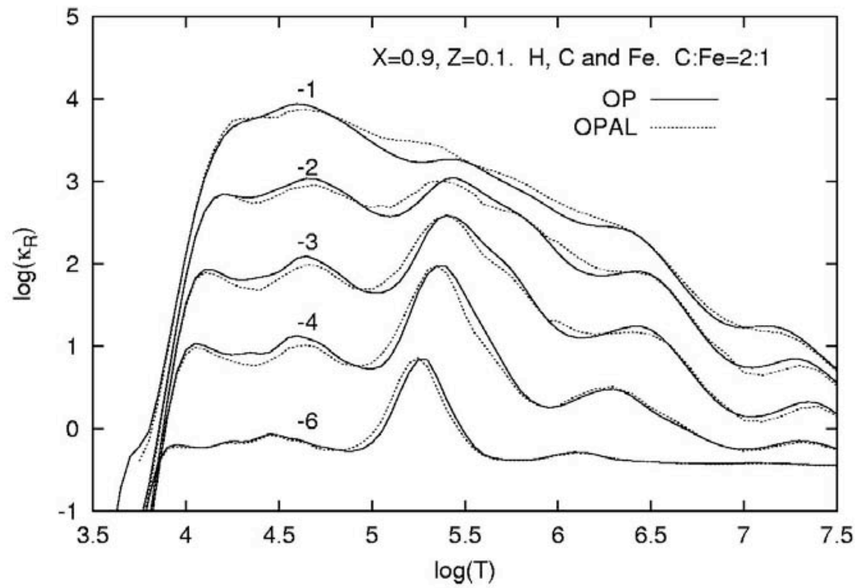


Figure 10. Comparisons of $\log(\kappa_R)$ from OP and OPAL for an iron-rich mixture: $X = 0.9$, $Z = 0.1$ and C:Fe=2:1 by number fraction. Curves are labelled by values of $\log(R)$.

(Log κ_R vs. Log T) at Log R = ρ / (T/ 10^6)^3

RADIATIVE ACCELERATION

Given BB radiative flux F(r) at depth r in a star with T_{eff} and radius R_* , the radiative acceleration of element k is

$$g_{rad}(r) = (\frac{1}{c})(\frac{M}{M_k})\kappa_R \gamma_k F(r), \quad (1)$$

where κ_R is the Rosseland mean opacity at temperature T and density ρ at r, and γ_k is a dimensionless quantity representing the ratio of the momentum-tranfer (mta) cross section to the total opacity cross section per atom

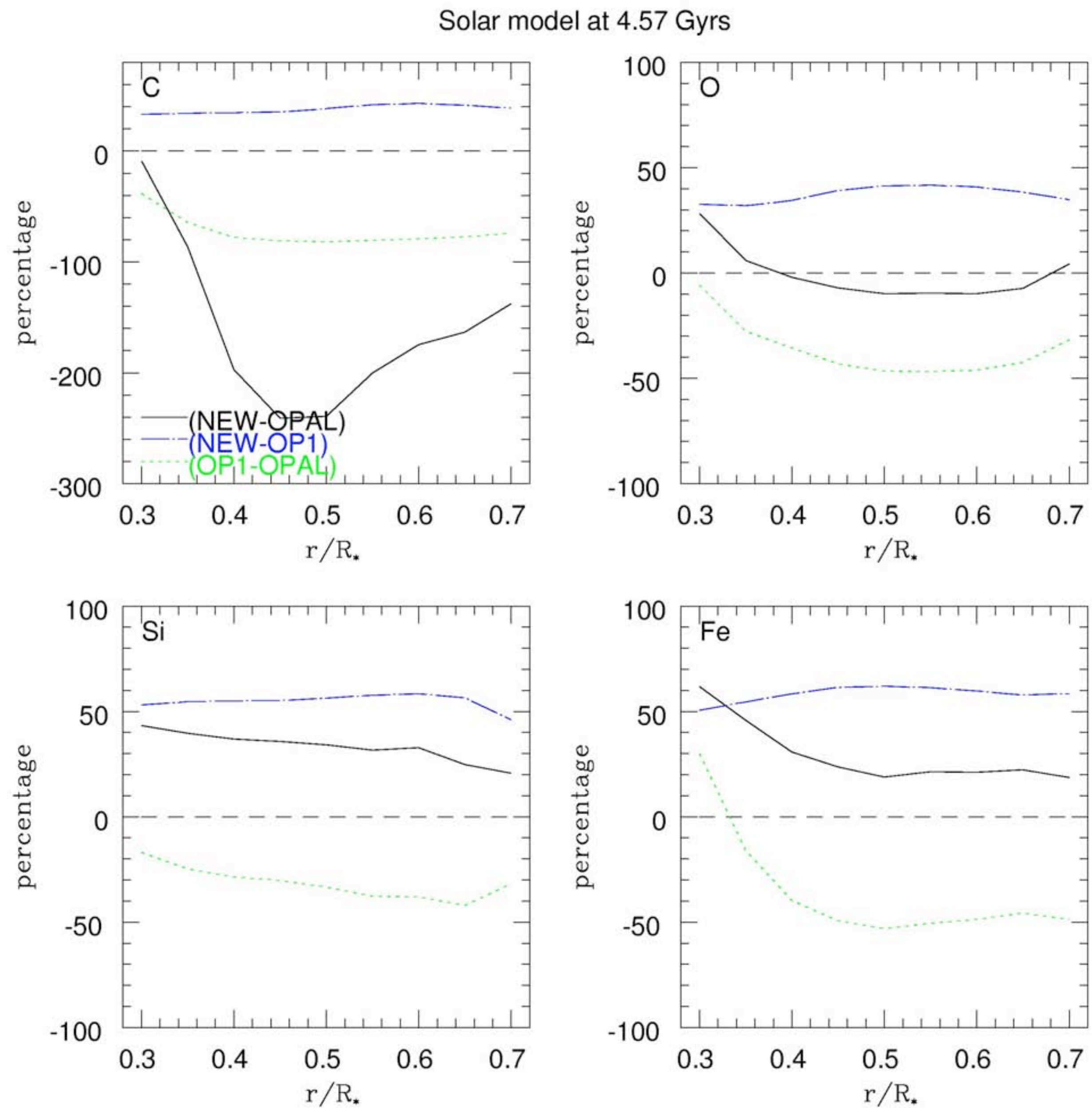
$$\gamma_k = \int \frac{\sigma_\nu^{mta}(k)}{\sigma_\nu(tot)} f_\nu d\nu, \quad (2)$$

where

$$f_\nu = \frac{(dB_\nu/dT)}{(dB/dT)}. \quad (3)$$

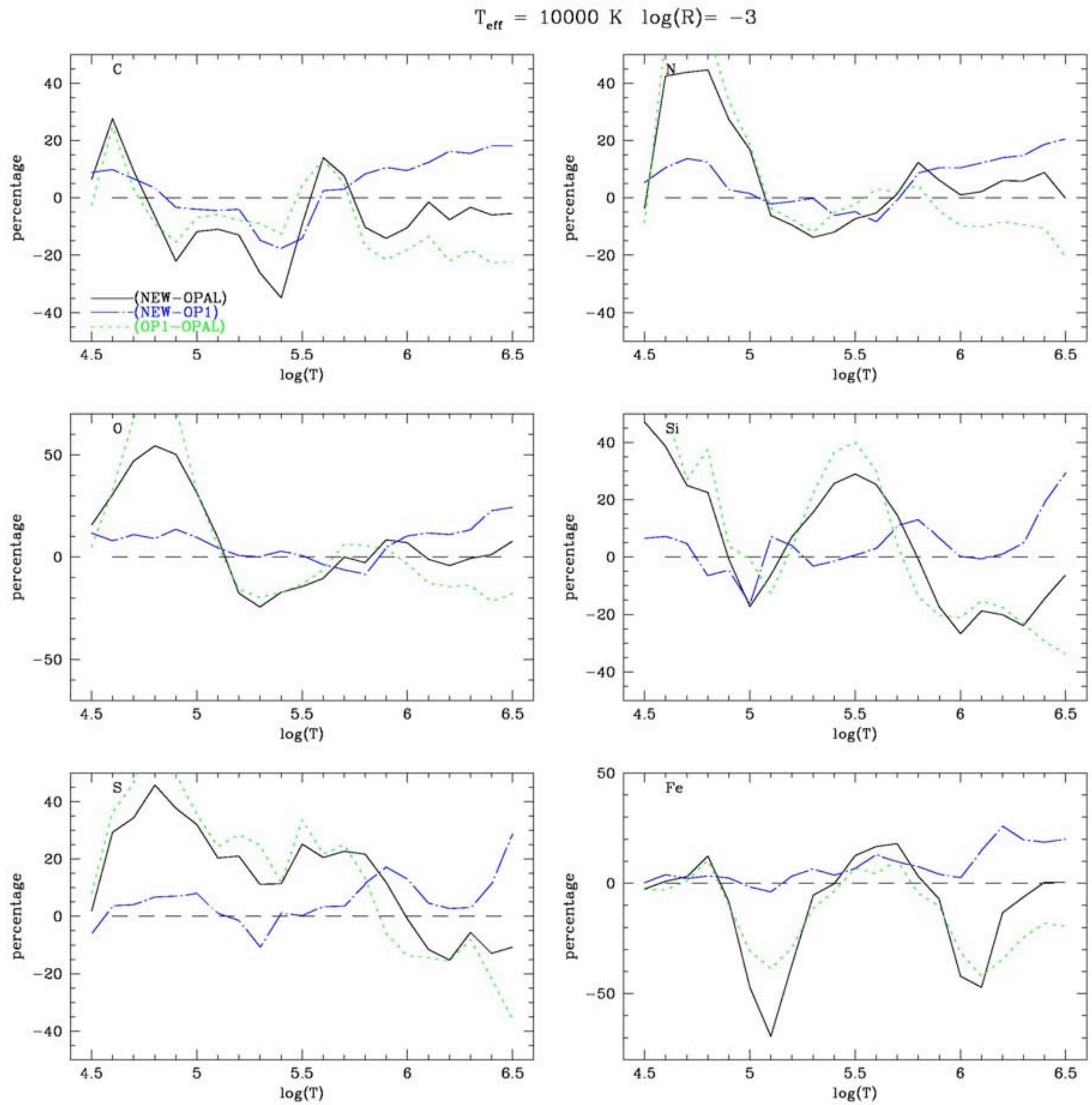
γ_κ is a measure of the specific opacity of element k relative to the total opacity, therefore much more sensitive to resolution and accuracy of atomic data than the Rosseland mean.

OP vs. OPAL → % Differences in g_{rad} for the Sun



Delahaye & Pinsonneault (2005, ApJ in press)

OP vs. OPAL → % Differences in Radiative Accelerations



Delahaye & Pinsonneault (2005, ApJ in press)

New Solar Abundances (And Problems!)

- Latest determination of solar abundances (Asplund et.al. 2005) – measurements and 3D hydro NLTE models – yield

→ **30- 40% lower abundances of C,N,O,Ne,Ar**

- However, this disagrees with Helioseismology data (sound speed, BCZ, etc.), and

→ **would require the OP and OPAL opacities to be lower by about 10%; EOS has little effect (Bahcall et.al. 2004)**

Causes: Resolution

- Radiative acceleration g_{rad} or γ are more sensitive to resolution than the Rosseland mean opacities (RMO)
- Both OP and OPAL RMOs converge to 2% with 10^4 points, γ could differ by several factors depending on element and physical conditions
- OP data uses an adjustable mesh with better resolution

Causes: Accuracy of Atomic Physics

- Only a relatively small subset of OP atomic data is from the R-matrix calculations
- Both OP and OPAL data may not differ much in absolute accuracy
- New Calculations – Iron Project and Beyond
- Compare Close-Coupling R-matrix and other methods
- Verify results for fundamental atomic parameters for primary processes
- High precision atomic physics

Coupled Channel R-Matrix Theory vs. Distorted Wave

Coupled Channel Theory

The wavefunction expansion, $\Psi(E)$, for a total spin and angular symmetry $SL\pi$ or $J\pi$, of the (N+1) electron system is represented in terms of the target ion states as:

$$\Psi(E) = A\sum_i \chi_i\theta_i + \sum_j c_j\Phi_j, \qquad (1)$$

where χ_i is the target ion wave function in a specific state $S_iL_i\pi_i$ or level $J_i\pi_i$, and θ_i is the wave function for the (N+1)th electron in a channel labeled as $S_iL_i(J_i)\pi_i\ k_i^2\ell_i(SL\pi)\ [J\pi]$; k_i^2 is the incident kinetic energy. In the second sum the Φ_j's are correlation wavefunctions of the (N+1) electron system.

- Ab initio treatment of **important** atomic processes with the same expansion: Eq.(1)
- Electron impact excitation, radiative transitions, and a **self-consistent and unified treatment of photoionization and (e + ion) recombination, including radiative and dielectronic (RR+DR) (Nahar, Zhang, Pradhan)**

All **significant** effects may be included

- Infinite series of resonances are considered

Distorted Wave Theory
Central Field Approximation

- **Includes only initial and final channels in Eq. (1); no summation**
- **Neglects channel coupling**
- **Resonance states (intermediate channels) NOT included in wavefunction expansion**
- **Resonances may be considered indirectly in the Isolated Resonance Approximation**
- **Finite number of resonances with n-extrapolation**

Accuracy AND Completeness: New Opacities Calculations

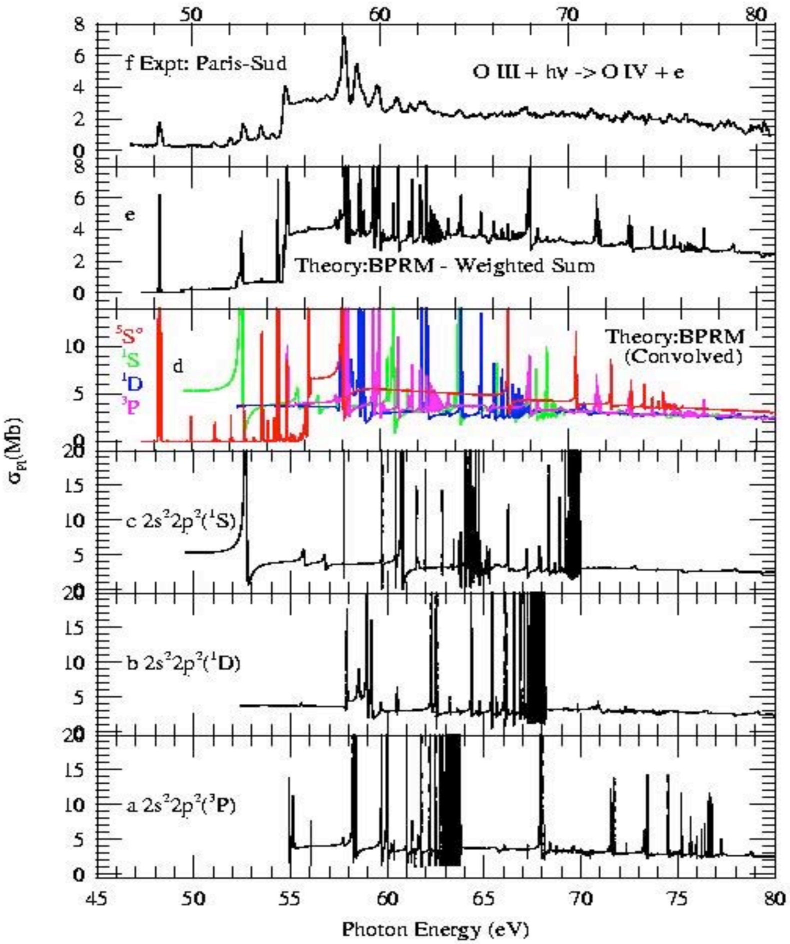
- Aim for high precision **first**, then completeness
- Benchmark state-of-the-art theoretical calculations with experiments for

  Photoionization - Accelerator based Advanced Light Sources (Reno/Berkeley, Aarhus, Paris)

  Recombination - Heavy ion storage rings (Heidelberg, Stockholm)

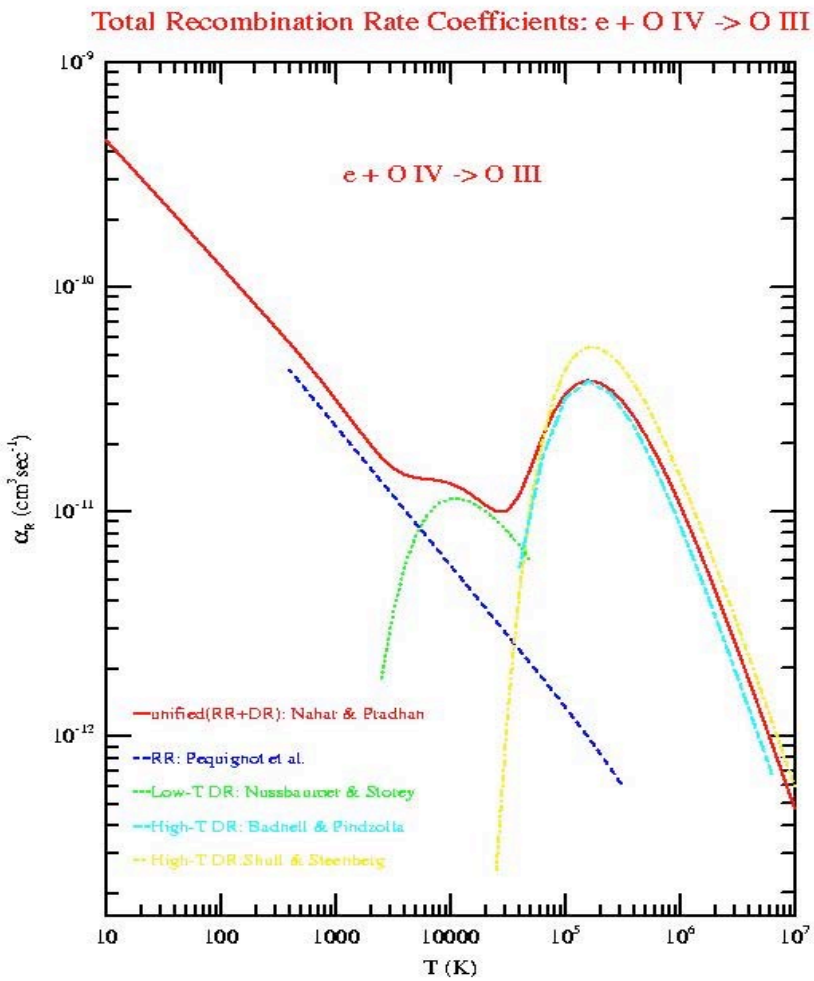
  Electron-Ion Scattering - Electron Beam Ion Traps (Livermore, NIST)

Photoionization of O III
Comparison of R-Matrix Theory (Nahar 2003) and Experiment (Bijeau etal 2003)



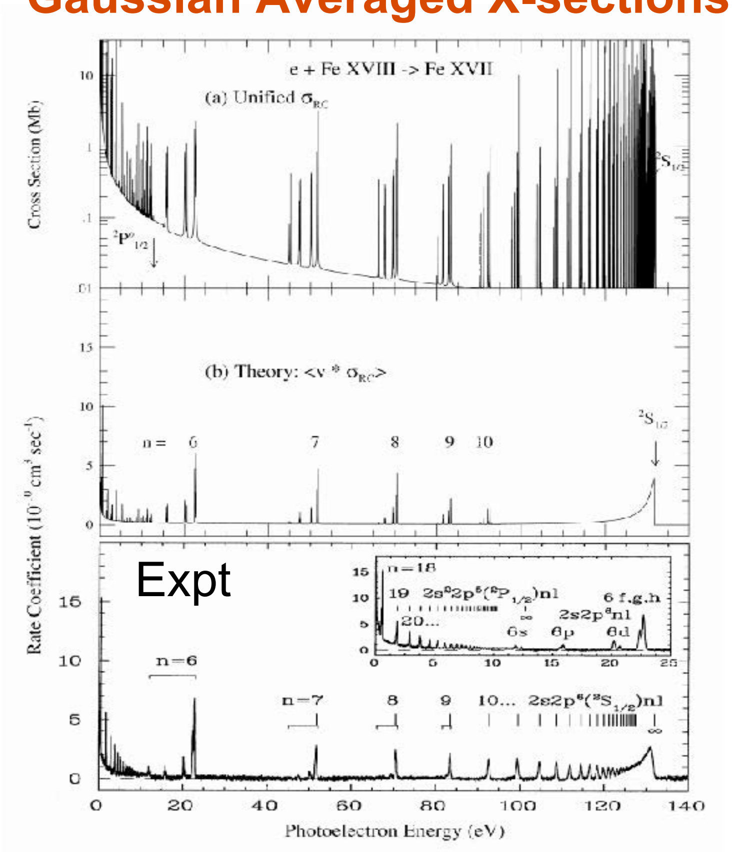
Experiment includes the ground state and metastable states of O III in the beam

Unified (e+ion) Recombination Rate Coefficient (RR+DR)

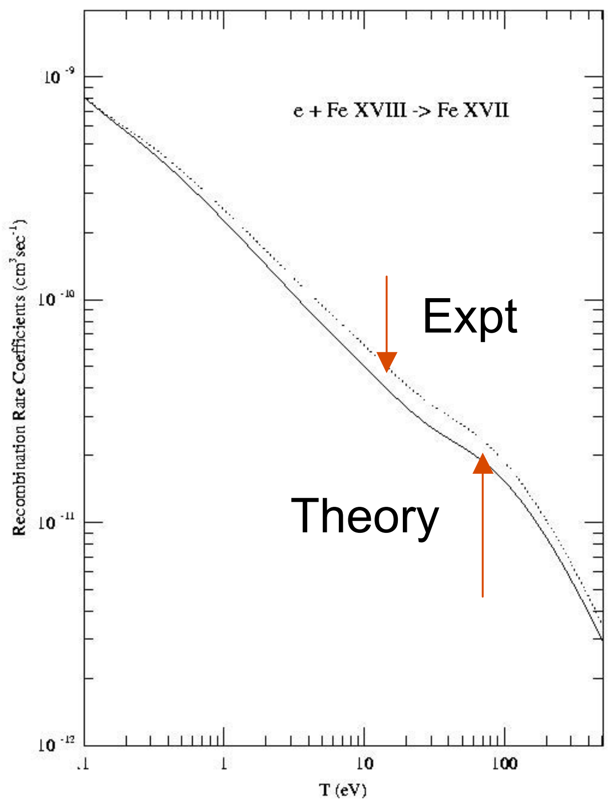


Unified (e+ion) recombination: R-Matrix Theory and Experiments

Gaussian Averaged X-sections



Maxwellian Averaged Rate



Rates agree to < 20%

Theory: Pradhan, Nahar, and Zhang (ApJL, 549, L265, 2001)

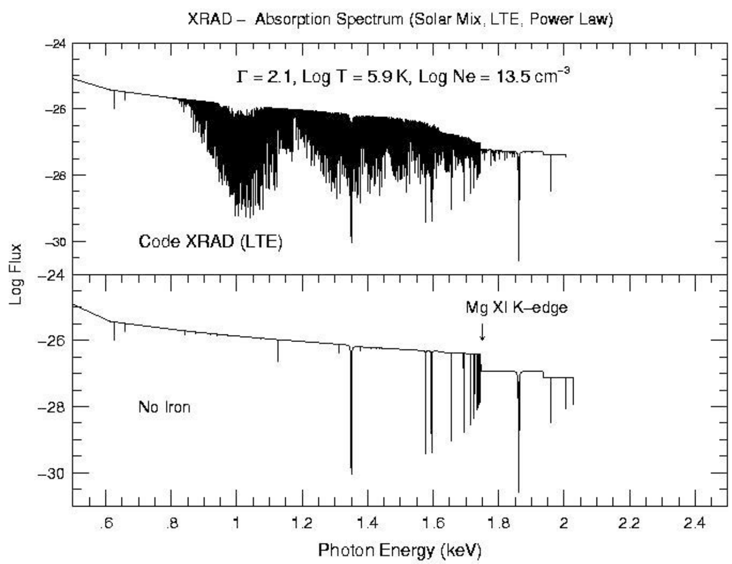
Expt: Savin et.al. (ApJS, 123, 687, 1999)

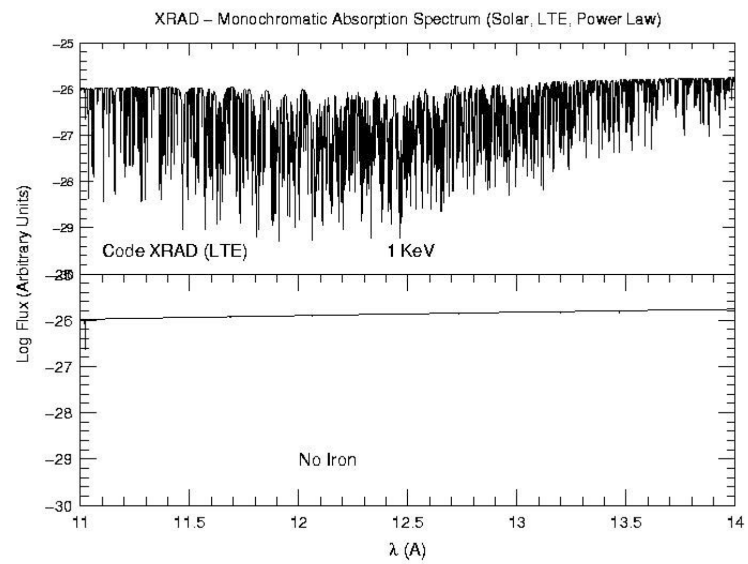
Monochromatic Opacities

- Experimental verification of
  → Cross sections and transition rates
  → Monochromatic opacity/transmission spectra of elements
- Astrophysical verification with observed spectra

Code XRAD – Theoretical X-ray Absorption Spectrum
The Opacity Project and The Iron Project Data

(Pradhan 2004)





Power-law radiation field (NOT Blackbody),
Monochromatic opacities and spectrum for arbitrary mixtures

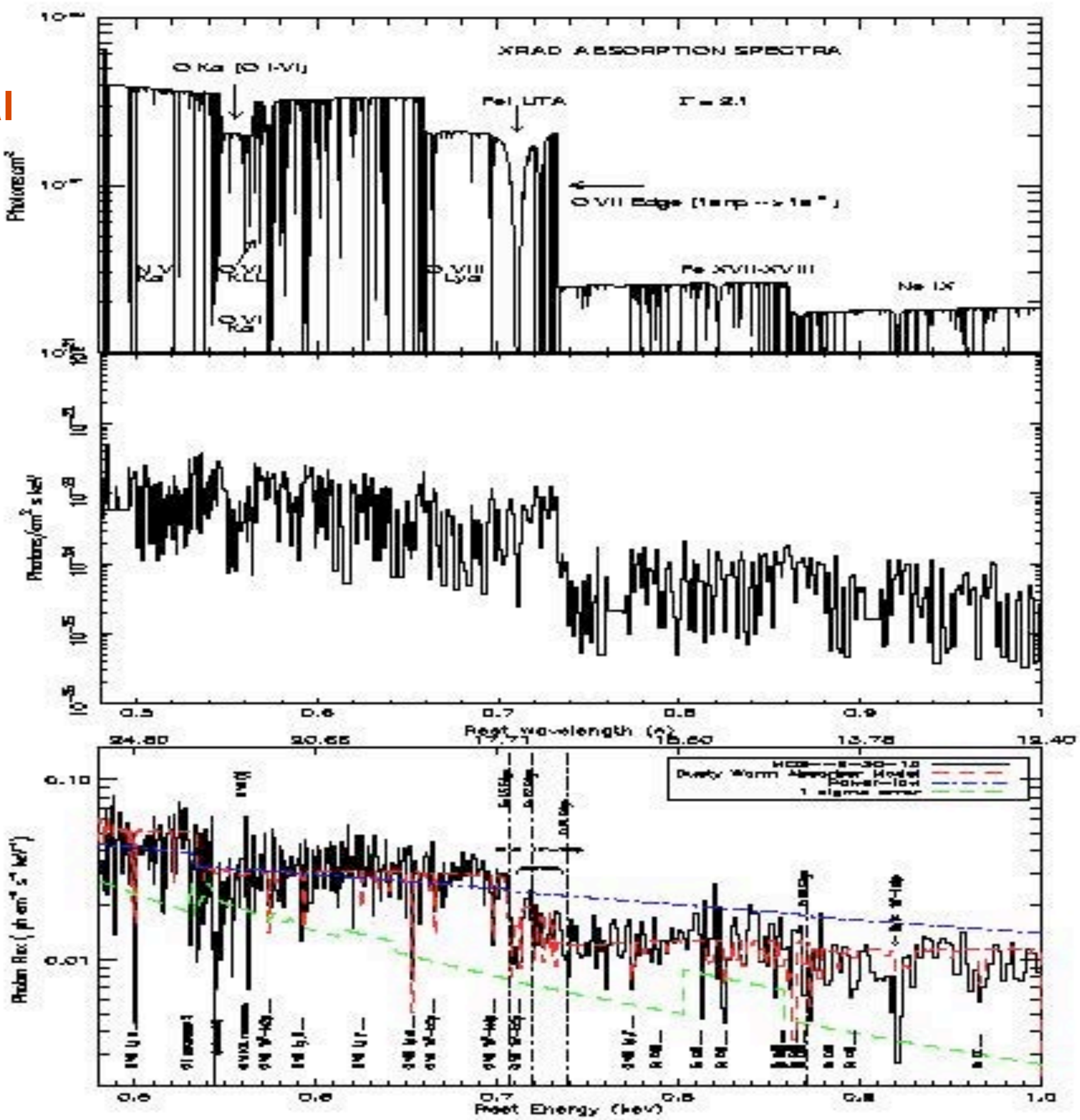
Mono X-ray Opacities: Modeling The Spectrum of AGN MCG-6-30-15

Black Hole Candidate: Relativistic Gravitational Broadening ?

Code XRAD (Pradhan 04)

Convolved with XSPEC

Chandra Spectrum (Lee et.al. 2001)

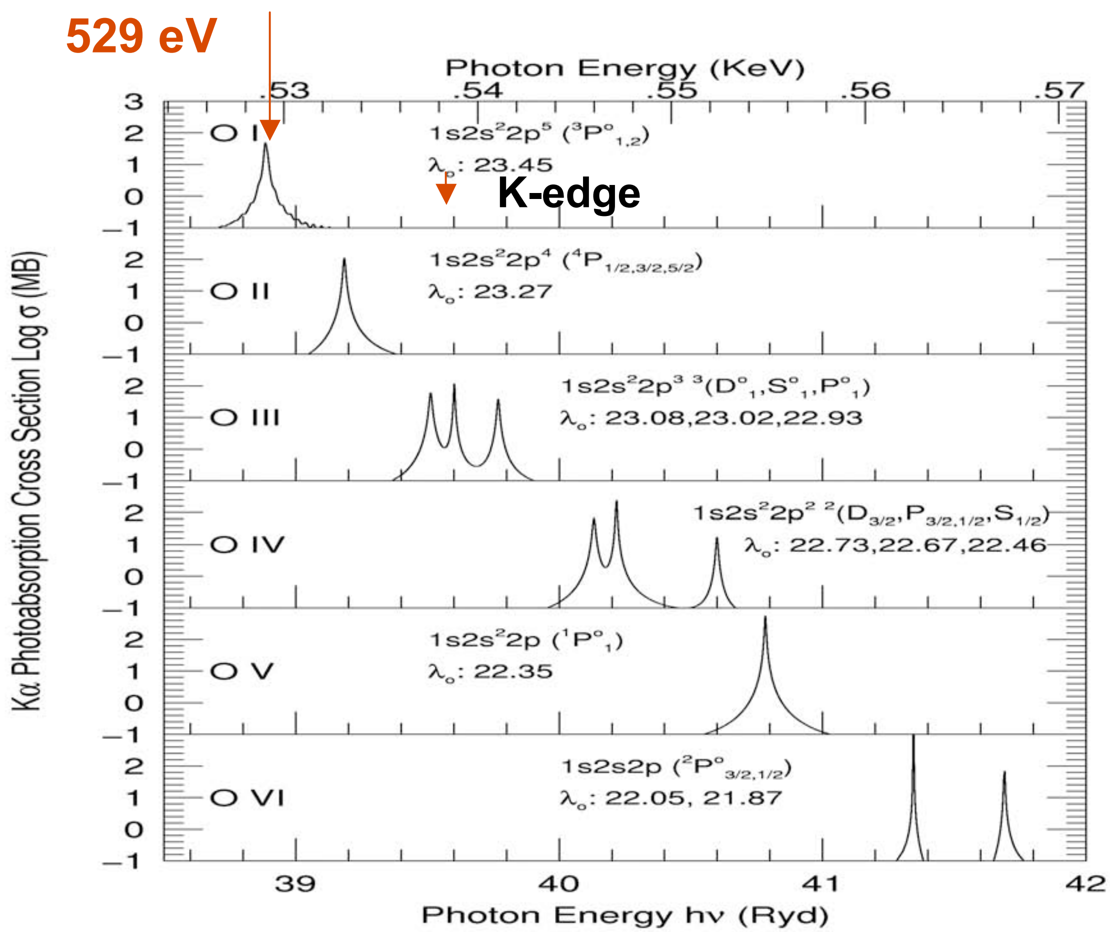


NANOSPECTROSCOPY
Computational Nanoscience at Fundamental Atomic and Molecular Scales (OSU)

- **Nanobiomedicine and Nanomaterials**
- **Broadband (indiscrimate!) imaging yields pictures, but not detailed nanoscopic information**
- **Spectroscopy is the most powerful tool**

  "A spectrum is worth a thousand pictures"
- **Paradigm shift from imaging to spectroscopy, such as occurred in astronomy**
- **Spectroscopy should be far more efficient with reduced radiation exposure by targeting spectral features in atoms and molecules**

Resonance Peaks in X-Ray Photoabsorption By Oxygen



Resonance in neutral O at 0.529keV; X-ray absorption cross section is higher by factor of up to 100 than at other energies

AVOID X-RAYS AT 529 eV → ~ 100 TIMES MORE DAMAGE TO HUMAN BODY !!

Pradhan, Nahar, Delahaye, Chen, Oelgoetz (2003)

Spectral ‘Windows’ in X-ray opacities

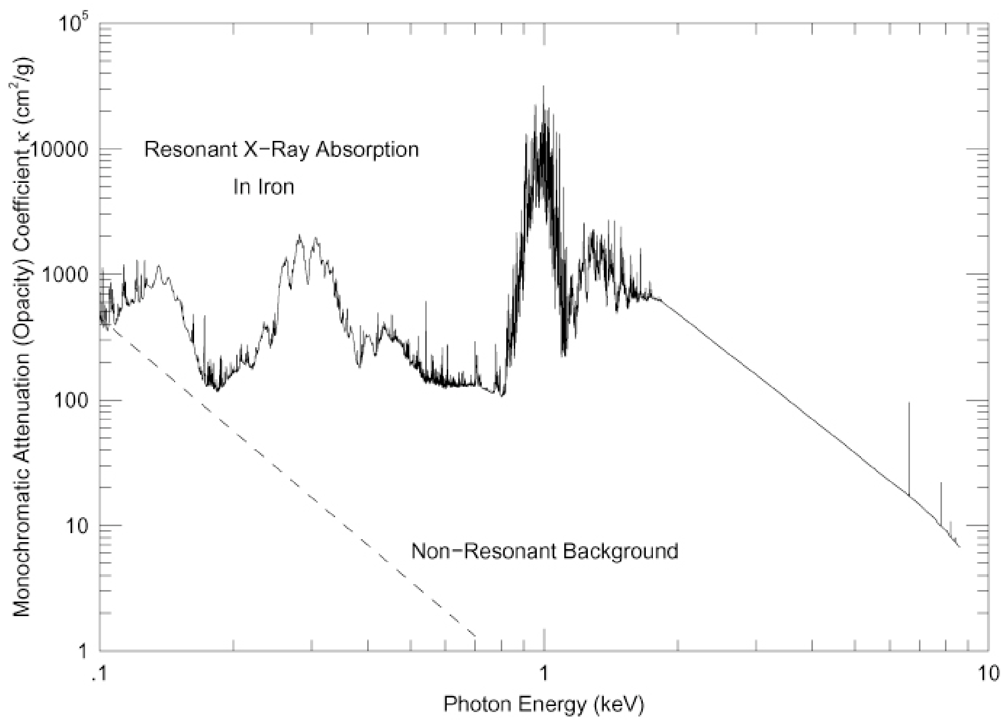
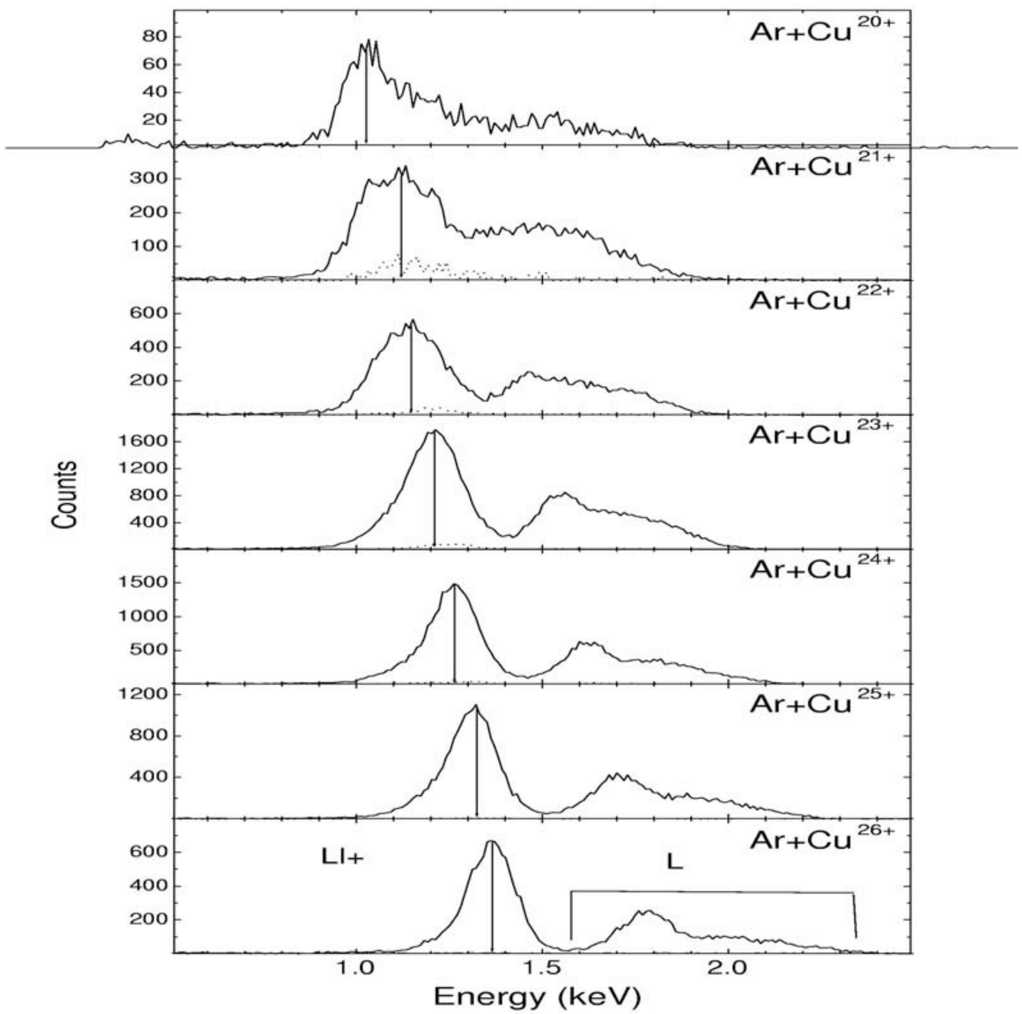


Fig. 1. The enhancement in X-ray photo-absorption in iron due to low energy resonance complexes. Compared to the non-resonant background, the attenuation coefficients may be up to several orders of magnitude higher, particularly in specific 'spectral windows' such as the one at 1 KeV due to L-shell excitations. Heavier elements will have such features at much higher energies.

Lighter ‘biogenic’ elements (H,C,N,O) have far lower absorption coefficient at high energies; beyond the K-edge, cross section ~ E-3.
X-rays are absorbed by iron and heavier elements with orders of magnitude higher efficiency at energies of resonance-arrays.

Experiment: X-Ray Fluorescent Emission "Spectral Windows" From Copper



Preliminary results from collaborators using the Pelletron: Heavy ion Accelerator at the Tata Institute For Fundamental Research, Mumbai, India (A. Kumar & L. Tribedi, private communication)

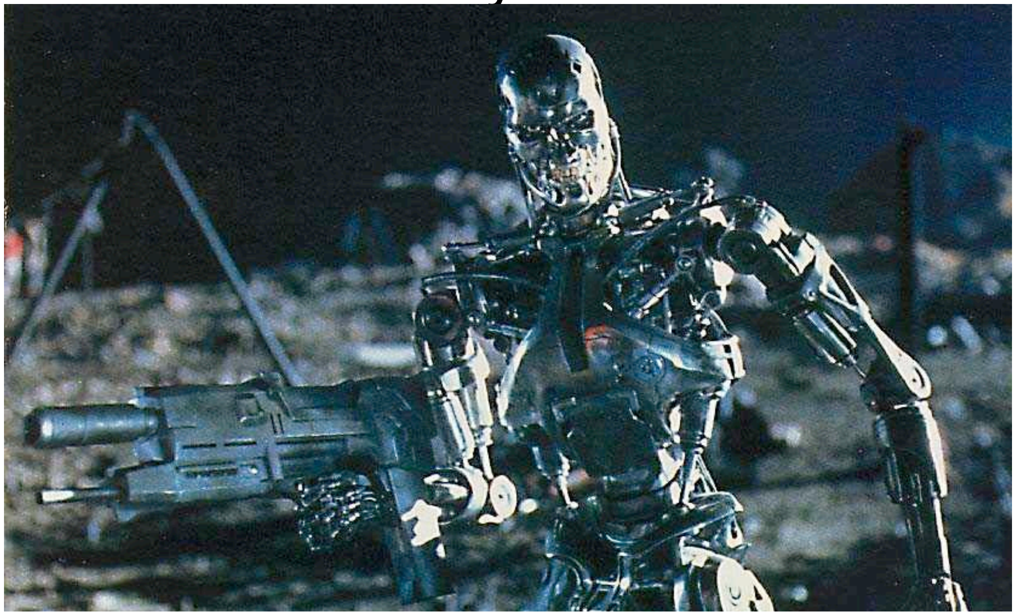
More experiments needed to locate peak emission windows

Conclusion

- Definitive opacities with state-of-the-art atomic physics have not yet been computed (EOS ?)
- Calculations are needed for heavy elements, **Iron and beyond**, including relativisitic effects using Breit-Pauli or Dirac R-matrix codes
- Collaboration with LANL, LLNL might be desirable to compare detailed opacities
- Nanotechnology, fusion, and other applications next generation of AM codes

New Computational Technology For Atomic and Molecular Physics

- TENSOR CONTRACTION ENGINE (TCE) for automatic formula derivations and parallel implementation of any given model of wave function theory.
  - Expediency
  - Optimization & Parallelization
  - Maintainability & portability
  - Extensibility



"It doesn't feel pity, or remorse, or fear."
The Terminator

(And has no sense of humor)